

Spin polarization anisotropy in a narrow spin-orbit-coupled nanowire quantum dot

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Single and two-electron systems confined in nanowire quantum dots are studied in the context of spin-orbit coupling effects. Anisotropy of the spin-orbit interaction is discussed in terms of the system geometry and orientation of the external magnetic field. We find that in the limit of strong lateral confinement the electron spin becomes well defined in spite of the presence of spin-orbit coupling. We present an analytical solution for the one-dimensional limit and study its applicability for finite thickness nanowires by comparing the results with a full three-dimensional calculation. The present results are confronted with the recent measurements of the effective Landé factor anisotropy in InSb nanowire quantum dots [S. Nadj-Perge *et al.*, Phys. Rev. Lett. 108, 166801 (2012)].

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I. INTRODUCTION

There is a growing interest in gated semiconductor nanowires in the context of possible applications for spin-operating devices.^{1–4} These structures provide a good basis for creation of small quantum dots induced by external voltages. Energy spectra of such dots as determined⁵ by transport spectroscopy bear distinct signatures of strong spin-orbit (SO) interaction which results from the structure inversion asymmetry (Rashba SO coupling⁶) or the bulk inversion asymmetry (Dresselhaus SO interaction⁷). SO coupling mixes spin and orbital degrees of freedom and opens the possibility of fully electrical control of the electron spin,^{1–4,8,9} allow for electron spin relaxation mediated by phonons,^{10,11} and introduce anisotropic corrections to spin SWAP process.¹²

The SO coupling opens avoided crossings⁵ in the quantum dot energy spectra as function of the external magnetic field (\mathbf{B}). The width of the avoided crossings between energy levels of different spin states depends on the orientation of \mathbf{B} vector. The dependence reveals the anisotropy of the SO interaction.^{3,13–15} Moreover, the mixing of the spin states by SO coupling determines an effective Landé factor (g-factor) and its anisotropy¹⁶ in function of the magnetic field orientation. In a nanowire quantum dots the effective g-factor was recently measured^{2,3} in electric dipole spin resonance (EDSR) experiments for a two-electron spin-blocked configuration. The anisotropy of SO interaction is a relevant issue for spin qubit manipulation¹ as well as for helical spin liquids¹⁷ which in the proximity of a superconductor can be used for observation of Majorana fermions.¹⁸

It is well known, that in the presence of SO coupling the electron spin can be well defined in the stationary eigenstates only for equal Rashba and Dresselhaus SO coupling constants.¹⁹ This fact was exploited in a proposal of nonballistic spin field effect transistor¹⁹ and for prediction²⁰ of persistent spin helix.²¹ In the present work we demonstrate that in the limit of strong lateral

confinement the electron spins become well defined in the direction perpendicular to the wire axis and the external electric field vector in spite of the presence of the pure Rashba coupling. In a general case, we show that depending of the external magnetic field orientation the electron spin states can be strongly mixed or an almost complete spin polarization is obtained.

For a description of narrow nanowires a one-dimensional model is commonly used.²² In the present work we present an analytical form of eigenstates for this approximation. The analytical form of the SO-coupled wave functions explains a different strengths of the spin-splittings for varied orientation of the magnetic field. We study applicability of the one-dimensional model for a finite radius nanowire by comparing its results with three-dimensional calculation for various geometries of nanowire quantum dot. We relate our results in the two-electron regime to the measurements of effective g-factor on an InSb nanowire quantum dot in the EDSR experiment of Ref. 3.

II. THEORY

We consider single-electron nanowire quantum dot described by the three-dimensional Hamiltonian,

$$H = \frac{\hbar^2 \mathbf{k}^2}{2m^*} + V(\mathbf{r}) + H_{SO} + \frac{1}{2}g\mu_B \mathbf{B} \cdot \boldsymbol{\sigma} + |e|\mathbf{F} \cdot \mathbf{r}, \quad (1)$$

where $\mathbf{k} = -i\nabla + e\mathbf{A}/\hbar$ with the gauge $\mathbf{A} = B(z \sin \phi, 0, y \cos \phi)$. The magnetic field is aligned in the xy -plane with an angle ϕ between the \mathbf{B} and x -axis – in such a case the Zeeman term stands $\frac{1}{2}g\mu_B \mathbf{B} \cdot \boldsymbol{\sigma} = \frac{1}{2}\mu_B g B(\sigma_x \cos \phi + \sigma_y \sin \phi)$. We account for Rashba SO coupling $H_{SO} = \alpha_0 \frac{\partial V(\mathbf{r})}{\partial \mathbf{r}} \cdot (\boldsymbol{\sigma} \times \mathbf{k})$ as the main SO interaction type in the [111] grown InSb nanowires.³ $V(\mathbf{r})$ stands for the confinement potential which we take in a separable form $V(\mathbf{r}) = V_l(y, z)V(x)$ where $V_l(y, z)$ is a 400 meV deep two-dimensional circular quantum well of

radius R , and $V(x)$ is a infinite quantum well with width L . We assume electric field $\mathbf{F} = (0, 0, F_z)$ with non-zero component in the z -direction (perpendicular to the axis of the wire) due to the gating of the nanowire.¹⁻⁴ For this form of the electric field $H_{SO} = \alpha(\sigma_x k_y - \sigma_y k_x)$ where $\alpha = \alpha_0 F_z$.

We solve the Schrödinger equation using finite difference method on a grid employing method previously used for self-organized quantum dots¹⁴ where the single-electron solutions are found in basis constructed from one-dimensional spin-orbitals.

The two-electron system is described by the Hamiltonian,

$$H = h_1 + h_2 + \frac{e^2}{4\pi\epsilon_0\epsilon|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (2)$$

and calculation is performed within configuration interaction scheme which treats the Coulomb interaction in exact manner including electron-electron exchange and correlation.

We adopt material parameters²⁴ for InSb, namely : $m^* = 0.014m_0$, $g = -51$, $\epsilon = 16.5$, and $\alpha_0 = 5 \text{ nm}^2$. In the bulk of the paper we choose $F_z = 50 \text{ kV/cm}$ which results in SO interaction strength $\alpha = 25 \text{ meVnm}$. Unless stated otherwise we take $L = 300 \text{ nm}$.

III. RESULTS

A. Single electron in a finite thickness nanowire quantum dot

Lowest part of the energy spectrum of the single-electron quantum dot is presented in Fig. 1. In the absence of the magnetic field all the levels are Kramer's doublets. We include residual magnetic field with $B = 5 \text{ mT}$ and check the spin polarization along the magnetic field direction (calculated as $\langle s_B \rangle = \langle s_x \rangle \cos(\phi) + \langle s_y \rangle \sin(\phi)$). In Fig. 2(a) we present that the spin polarization undergoes oscillatory changes as function of \mathbf{B} orientation. This reflects the presence of the easy and hard spin polarization axes in the system. For the magnetic field oriented perpendicular to the nanowire axis the spin is easily polarized – taking values close to $1 [\hbar/2]$. On the other hand for \mathbf{B} oriented along the wire the $\langle s_B \rangle$ is around $0.885 \hbar/2$. The amplitude of the oscillations depends on the nanowire radius (compare the curves in Fig. 2(a) for three values of R) and the oscillations are the strongest for narrow nanowire with $R = 10 \text{ nm}$. Let us set $\phi = 90^\circ$ and further inspect the spin polarization. In Fig. 2(b) we plot mean value of the spin- y component in function of the wire radius R . We observe that as the wire becomes narrower the spin polarization becomes almost complete (i.e., $1 - \langle s_y \rangle 2/\hbar < 10^{-4}$ for $R = 1 \text{ nm}$) despite the presence of the SO coupling. On the other hand as the wire becomes wider the spin-polarization drops with the slope of the curves in Fig. 2 depending on the SO strength α .

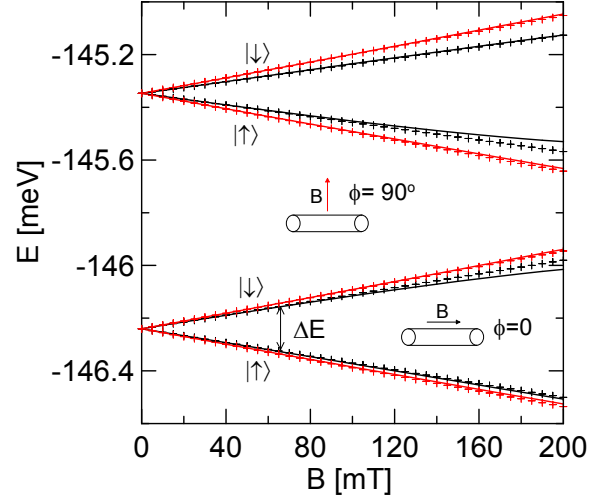


FIG. 1. (color online) Single-electron energy spectrum for the SO coupled nanowire quantum dot with radius $R = 50 \text{ nm}$ and SO interaction strength $\alpha = 25 \text{ meVnm}$ plotted with lines for two orientations of the magnetic field. The crosses are the results obtained from asymptotic one-dimensional solution – see text. With $|\uparrow\rangle$ and $|\downarrow\rangle$ we mark the spin-polarization of the states parallel and antiparallel to the magnetic field respectively as found without SO coupling.

When the magnetic field is increased it splits the doublets – see the energy levels in Fig. 1. The energy splittings obtained for magnetic field perpendicular to the nanowire axis (red curves in Fig. 1) are stronger than the ones obtained for magnetic field parallel to the nanowire axis (black curves in Fig. 1). In the following we explain this observation.

B. Asymptotic solution (1D limit)

When the wire becomes narrow the energy of the states excited in the radial direction (in our case the y and z directions) rises. It is reasonable then to inspect the case where the radial degrees of freedom are decoupled from the longitudinal one (the x -direction). Such a system is described by the one-dimensional Hamiltonian,^{22,23}

$$h_{1D} = \frac{\hbar^2 k_x^2}{2m^*} + V(x) - \alpha \sigma_y k_x + \frac{1}{2} \mu_B g B (\sigma_x \cos \phi + \sigma_y \sin \phi), \quad (3)$$

where $k_x = -i \frac{\partial}{\partial x}$.

Generally, the analytical solution for a SO coupled confined systems are not known with the exception of a special case of equal strength of Rashba and Dresselhaus coupling described in Ref. 19. Here we note however that in the absence of the magnetic field ($B = 0$) the Hamiltonian (3) commutes with spin- y Pauli matrix and its eigenstates are the states with well defined spin in the y -direction. We find that for a quasi one-dimensional nanowire the spin-orbitals (where N stands for the or-

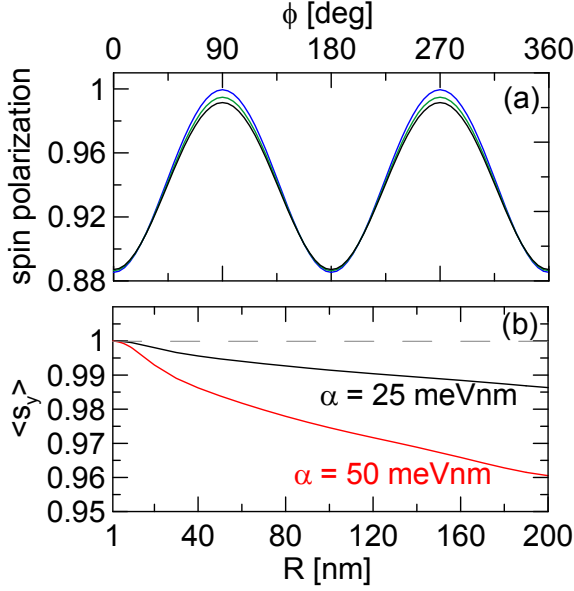


FIG. 2. (color online) (a) Mean value of the spin along magnetic field direction obtained for the nanowire with radius $R = 10$ nm (blue curve), $R = 50$ nm (green curve) and $R = 100$ nm (black curve). (a) mean value of the spin- y component for magnetic field aligned along y -direction in function of the nanowire radius R . (a) and (b) are obtained for $B = 5$ mT. Results for $\alpha = 50$ meVnm are obtained with $F_z = 50$ kV/cm.

bital quantum number and \pm for the spin polarization of the state) have the form,

$$\Psi_{N\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} \varphi_N(x) \exp \left[\pm \frac{i\alpha m^*}{\hbar^2} x \right], \quad (4)$$

where $\varphi_N(x)$ are spin-independent eigenstates of Hamiltonian (3) for $\alpha = 0$ and $B = 0$. The eigenenergies of the Hamiltonian (3) are $E_{1D} = E_{\alpha=0,N} + E_{SO}$ where $E_{SO} = -\alpha^2 m^*/(2\hbar^2)$ is the energy shift to the whole energy spectrum introduced by the SO interaction²⁵ and $E_{\alpha=0,N}$ is an energy level of the N 'th eigenstate obtained without SO coupling.

The magnetic field affects the energy levels of a strongly confined electron mainly through the Zeeman spin-splitting. To investigate its influence on the SO eigenstates with orbital excitation N let us diagonalize h_{1D} for $B > 0$ in a basis consisting of a degenerate pair Ψ_{N+} and Ψ_{N-} . The Hamiltonian matrix is

$$\begin{pmatrix} \langle \Psi_{N+} | h_{1D} | \Psi_{N+} \rangle & \langle \Psi_{N-} | h_{1D} | \Psi_{N+} \rangle \\ \langle \Psi_{N+} | h_{1D} | \Psi_{N-} \rangle & \langle \Psi_{N-} | h_{1D} | \Psi_{N-} \rangle \end{pmatrix}, \quad (5)$$

where the diagonal elements are defined as follows

$$\langle \Psi_{N\pm} | h_{1D} | \Psi_{N\pm} \rangle = E_{1D} \pm \frac{1}{2} g \mu_B B \sin \phi, \quad (6)$$

while the off-diagonal elements are

$$\begin{aligned} \langle \Psi_{N\pm} | h_{1D} | \Psi_{N\mp} \rangle = \\ \mp i \frac{1}{2} g \mu_B B \int |\varphi_N|^2 \left[\cos\left(\frac{2\alpha m^*}{\hbar^2} x\right) \mp i \sin\left(\frac{2\alpha m^*}{\hbar^2} x\right) \right] dx \cos \phi. \end{aligned} \quad (7)$$

Let us denote $\lambda_N \equiv \int |\varphi_N|^2 \cos(\frac{2\alpha m^*}{\hbar^2} x) dx$ and $\kappa_N \equiv i \int |\varphi_N|^2 \sin(\frac{2\alpha m^*}{\hbar^2} x) dx$.

The eigenstates of the matrix (5) are

$$E_{N\pm} = E_{1D} \pm \frac{1}{2} g \mu_B B \sqrt{1 - (1 - \lambda_N^2 + \kappa_N^2) \cos^2 \phi}. \quad (8)$$

The energy difference between the states depends on the orientation of the magnetic field (angle ϕ) as well as the parameters λ_N and κ_N that control strength of the anisotropy of the spin splittings for rotated magnetic field. For the symmetric infinite quantum well confinement along the wire (x -direction) we obtain,²⁷

$$\lambda_1 = \frac{\hbar^6 \pi^2 \sin(L\alpha m^*/\hbar^2)}{\alpha m^* L (\pi^2 \hbar^4 - \alpha^2 m^{*2} L^2)}, \quad (9)$$

and

$$\lambda_2 = \frac{4\hbar^6 \pi^2 \sin(L\alpha m^*/\hbar^2)}{\alpha m^* L (4\pi^2 \hbar^4 - \alpha^2 m^{*2} L^2)}, \quad (10)$$

and $\kappa_1 = \kappa_2 = 0$ for the two lowest orbital excited states. The λ_N depends on the nanowire length and the SO strength. In Fig. 3 we present the λ_1 parameter in function of L and α . With the light-green dashed curve we depict the SO length $l_{SO} = \hbar/(m^* \alpha)$. We observe that λ_1 drops quickly when the length of the dot becomes greater than SO length. The shape of the λ_1 dependence on the SO strength for different quantum dot lengths is presented in Fig. 3(b) showing that the SO effects strongly depends on the quantum dot geometry and that λ_1 goes to 1 for vanishing SO coupling

The smaller λ_N is the stronger effect of SO coupling are. In particular for the magnetic field parallel to the nanowire axis the energy of the spin splitting is $E_S = g \mu_B B \lambda_N$. Consequently the splitting can even go to 0 due to strong mixing of the spin states by the SO interaction (the light blue region in Fig. 3(a)).

When the magnetic field is aligned in the direction perpendicular to the nanowire axis, i.e. $\phi = 90^\circ$ or $\phi = 270^\circ$ the off-diagonal elements of matrix (5) vanish and the energy levels are split by Zeeman energy with the bulk value of the g-factor. This is the reason for stronger spin splittings of the red curves in Fig. 1. For this configuration the spin-orbitals are separable into spin and orbital parts despite the presence of SO interaction and they have exact form of Eq. (4). For any other orientation of the magnetic field the off-diagonal elements mix the eigenstates (4). This results in decreasing the spin splittings by the SO interaction by the amount that depends on the λ_N and κ_N parameters – the spatial extent of the

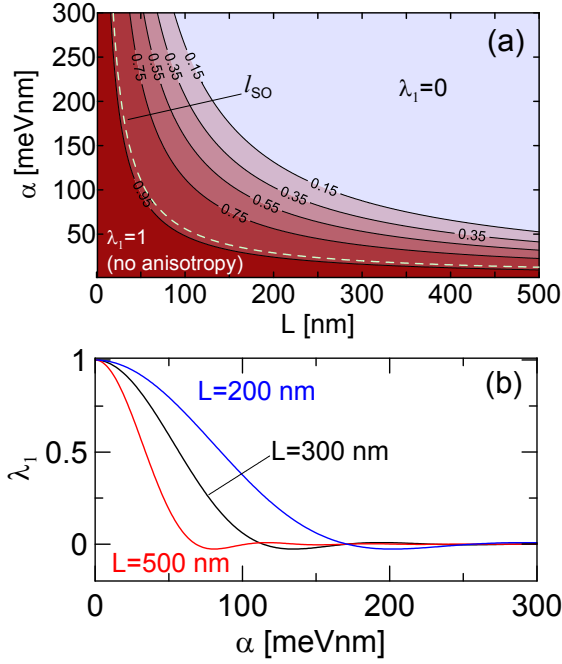


FIG. 3. (color online) Parameter λ_1 in function of dot length L and SO coupling strength α . (b) cross-section of (a) for three different dot lengths L .

wave function along the nanowire and the strength of the SO coupling. Moreover the electron spin is no longer well defined as the wave function is not separable into spin and orbital degree of freedom.

We plot the energy spectrum obtained from Eq. (8) (shifted to match the energies obtained in the three-dimensional calculation at $B = 0$) with the crosses on Fig. 1. The spin splitting obtained from the one-dimensional model well describes the results of the three-dimensional calculation. The only discrepancy is visible for the energy levels of the first and the second excited states for $B > 100$ mT which is due to mixing of this two states by the SO interaction.

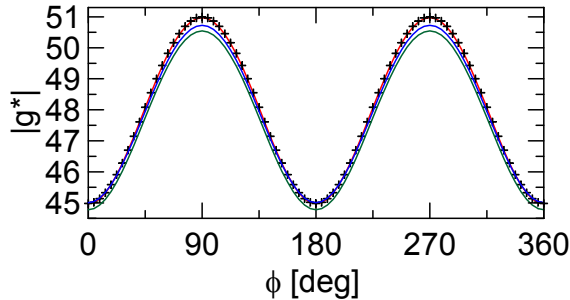


FIG. 4. (color online) Effective g-factor obtained for a nanowire with $R = 10$ nm (red curve), $R = 50$ nm (blue curve) and $R = 100$ nm (green curve) and from the one-dimensional model (black crosses). Results are obtained for $B = 100$ mT.

As the magnetic field is rotated between the easy and hard axes the spin-polarization of the states changes which results in changes of the spin-splitting strength. The latter term in Eq. (8) introduces Zeeman energy splitting between the energy levels of the two states. We can see that

$$g^* = g\sqrt{1 - (1 - \lambda^2 + \kappa^2)\cos^2\phi} \quad (11)$$

is an effective g-factor that is dependent on the orientation of magnetic field with the angle ϕ . With crosses in Fig. 4 we plot effective g-factor as obtained from Eq. (11) along with the values obtained in the three-dimensional calculation (calculated as $g^* = \Delta E/\mu_B B$, where ΔE is the energy difference between the energy of first excited state and the ground-state – see Fig. 1) for different nanowire radii. For the nanowire radius $R = 10$ nm they match perfectly. For the other two values of the R the shape of the dependence holds, only the amplitude is different, with the biggest discrepancy for the wide nanowire with $R = 100$ nm.

C. Two-electron results

The anisotropy of g-factor in the two-electron regime is extracted from the slopes of resonance lines in EDSR experiments on double quantum dots.^{2,3} Figure 5(a) presents two-electron energy spectrum of weakly coupled quantum dots in a nanowire obtained in the three-dimensional calculation for the nanowire with radius $R = 30$ nm. Results for the magnetic field oriented along the nanowire axis with $\phi = 0$ (perpendicular to the nanowire with $\phi = 90^\circ$) are plotted with solid (dotted) curves. The confinement potential includes now a potential barrier of 60 nm width that separates the electrons in adjacent dots both of 120 nm width. At $B = 0$ the ground-state is a singlet state ($|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$) split from the degenerate triplet states (see the inset to Fig. 5(a)). We tune the barrier height to 5 meV to match the singlet-triplet separation of $\simeq 5 \mu\text{eV}$ as measured in Ref. 3. At $B = 3$ mT an avoided crossing between the two lowest energy levels appears for $\phi = 0$ due to spin mixing by the SO interaction. After the anticrossing the magnetic field splits the energy levels of the two spin-polarized triplet states ($|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$) by the Zeeman energy. The blue and red curves in Fig. 5(a) whose energy does not change (after the anticrossing) with B are the singlet ($|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$) and triplet ($|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$) states with zero spin-component in the direction along the magnetic field. Those levels are split by exchange interaction²³ (additional splitting to those two energy levels occurs when the g-factor along the structure is not constant²⁻⁴).

The change of the magnetic field orientation (angle ϕ) results in: i) change in strength of the spin polarization of the triplet states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ which results in a change of the slope of the corresponding energy levels and ii) change in the exchange energy (spacing between energy

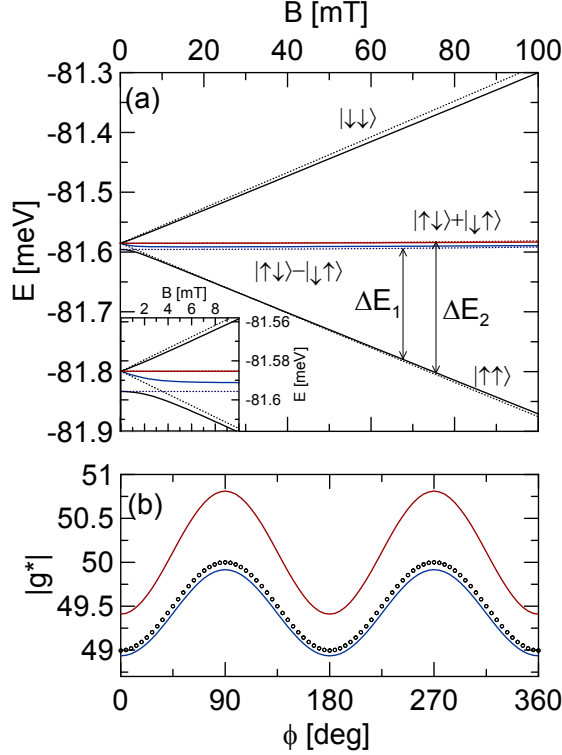


FIG. 5. (color online) (a) Two-electron energy spectrum of a coupled nanowire quantum dots with radius $R = 30$ nm. Solid curves present results for $\phi = 0$ and dotted curves for $\phi = 90^\circ$. With $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ we mark the spin configuration of the states parallel or antiparallel to the magnetic field as found without SO coupling. The inset presents the energy levels for low values of the magnetic field where the avoided crossing appears. (b) with the curves – effective g-factor calculated from the energy splittings between the ground-state energy level and the energy levels depicted with blue (ΔE_1) and red (ΔE_2) curves in (a) for $B = 200$ mT. The circles correspond to the effective one-electron g-factor as obtained from Eq. 11 (shifted down by 1) for a single quantum dot with length $L = 120$ nm.

levels of $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ states, plotted with blue and red curves in Fig. 5(a)). These two effects lead to a change of the effective g-factor which we calculate from the energy splittings between the ground-state and the first and second excited states and plot in Fig. 5(b) with the blue and red curves respectively. We find that the shape of both curves in Fig. 5(b) match the shape of the single-electron dependence presented in Fig. 4 only the amplitude of the oscillations is lower. As described by Eq. (11) for the single-electron case the amplitude of g-factor oscillations depends on the dot length. In the present case each of the coupled quantum dots has a length of $L = 120$ nm. The effective g-factor obtained for a *single* dot of this length as calculated from Eq. (11) is plotted with circles in Fig. 5(b). Obtained oscillations have similar amplitude to the ones obtained for the two-electron system. This suggest that the low amplitude

in the two-electron case results from the fact that each electron resides in a separate dot and the shape of the oscillations is controlled mainly by the single-electron spin polarization anisotropy.

The almost complete spin polarization occurring for the magnetic field oriented perpendicular to the nanowire results in closing of the the avoided crossing between the energy levels in the energy spectrum (see dotted curves in Fig. 5(a)). This finding is in agreement with the experimental results [3]. Also the shape of the g-factor dependence is similar to the one obtained in the experiment. In particular an agreement is obtained in the context of the slight change of the oscillation amplitude of the red and blue curves in Fig. 5(b). This difference in amplitudes is due to modification of the exchange energy that separates the energy levels of the singlet ($|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$) and triplet ($|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$) states by rotated magnetic field. However, the experimental dependence of the effective g-factor is shifted (with minima at $\phi = 124^\circ$ and $\phi = 304^\circ$) with respect to the present result. We performed calculations for quantum dots in a nanowire of larger radius ($R = 100$ nm) ruling out the possible orbital effects of the magnetic field as a reason for the shift. Our previous study¹⁴ indicates that any additional electric fields in the device activating additional Rashba terms, or the presence of Dresselhaus coupling would change the magnetic field angle for which the avoided crossing vanishes¹⁴ along with the shift of the effective g-factor angular dependence.

IV. SUMMARY AND CONCLUSIONS

In the present work we studied the anisotropy of the spin polarization in a narrow nanowire quantum dot in the presence of SO coupling. By the solution of the three-dimensional Schrödinger equation we showed that strength of the spin polarization under the presence of Rashba SO interaction depends on the orientation of the magnetic field and that there are hard and easy spin polarization axes as SO interaction tends to polarize spins in the direction perpendicular to the nanowire. For the magnetic field aligned in this direction the electron spin polarization can be nearly complete depending on the nanowire radius. We presented analytical solution for the one-dimensional limit and compared its results with the calculation for a finite thickness nanowire. The spin polarization anisotropy results in the effective g-factor dependence on the magnetic field orientation. The form of this dependence matches the one obtained in the experiment.

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